

Perfect state transfers by selective quantum interferences within complex spin networks

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We present a method that implement directional, perfect state transfers within a branched spin network by exploiting quantum interferences in the time-domain. That provides a tool to isolate subsystems from a large and complex one. Directionality is achieved by interrupting the spin-spin coupled evolution with periods of free Zeeman evolutions, whose timing is tuned to be commensurate with the relative phases accrued by specific spin pairs. This leads to a resonant transfer between the chosen qubits, and to a detuning of all remaining pathways in the network, using only global manipulations. As the transfer is perfect when the selected pathway is mediated by 2 or 3 spins, distant state transfers over complex networks can be achieved by successive recouplings among specific pairs/triads of spins. These effects are illustrated with a quantum simulator involving ¹³C NMR on Leucine's backbone; a six-spin network.

PACS numbers: 03.67.Lx, 03.67.Hk, 03.65.Xp, 76.60.-k

Quantum state control is essential in quantum information processing. In particular, the perfect state transfer (PST) between two-level systems (qubits) is one of the building blocks underlying quantum communications. Spin chains have been proposed as candidates for exploring short-distance communications [1] and XY-type (flip-flop) interactions tend to be essential to the efficiency of these quantum effects [2]. With such couplings, ideal quantum PSTs have been demonstrated in two and three spin chains [3, 4]. Perfect transfers, however, are still a challenge for larger spin chains –particularly for complex, branched spin networks. PST proposals to deal with these cases include engineering the spin-spin coupling intensities and/or the spin energies [4–7], as well as turning on-and-off the local couplings [3, 8]. A general feature of all these proposals is their requirement to access individual spins; either during the preparation of the quantum “hardware”, or during the transfer procedure. Either of these conditions is hard to implement with most present technologies. In fact, owing to the flexibility offered by active decoupling methods, heteronuclear nuclear magnetic resonance (NMR) presents one of the few scenarios where PSTs were demonstrated [3]. On the other hand, given the scarcity of heteronuclear qubits that can be simultaneously included in any one system, homonuclear-based methods could provide a much better platform for exploring PSTs and/or controlling other aspects of spin dynamics. Homonuclear NMR realizations of partial state transfers have actually been demonstrated; both by Mádi *et al.*, who explored a liquid-state linear chain system [9], and more recently by Cory *et al.*, who proposed measuring state transfers in a solid state sample with a linear coupling topology by relying on time-averaging techniques that requires simultaneous manipulations of individual spins [10]. Alternative theoretical proposals by Khaneja and Glaser [11] and by Fitzsimons and co-workers [12] allow for perfect transfers, by manipulating solely those spins at the end of linear Ising spin

chains.

Here, we introduce a different method for carrying out PSTs within a complex homonuclear system, that does not require any manipulation of individual spins. Instead, we exploit time domain quantum interferences that arise when spins evolve in the presence of non-commuting XY spin-spin coupling and Zeeman-type longitudinal Hamiltonians. It is shown that global manipulations with these interactions [13], can effectively turn on-and-off specific local couplings within the network, and achieve a full transfer of quantum information between distant qubits regardless of the spin network topology. We discuss some consequences of these ideas within the context of a liquid-state NMR “quantum PST simulator”.

Qubit-Selective Perfect Transfers in a Network.– Consider a spin network subject to the rotating-frame Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_Z + \hat{\mathcal{H}}_{\text{mix}} = \sum_i \hbar \Delta \Omega_i \hat{I}_i^z + \sum_{i \neq j} J_{ij} \left(\hat{I}_i^x \hat{I}_j^x + \hat{I}_i^y \hat{I}_j^y \right). \quad (1)$$

$\hat{\mathcal{H}}_Z$ is the longitudinal interaction of the spins defined by their $\Delta \Omega_i$ chemical shifts, and $\hat{\mathcal{H}}_{\text{mix}}$ is a suitable mixing Hamiltonian. We focus in particular on an XY mixing interaction, $\hat{\mathcal{H}}_{\text{mix}}^{XY}$, as it has been shown [4] that this allows PSTs to occur over 2 or 3 spins by setting every qubit/spin that belong to the channel to $|0\rangle = |\downarrow\rangle_z$ and the source spin in a quantum superposition $\alpha|0\rangle + \beta|1\rangle$, where $|1\rangle = |\uparrow\rangle_z$. Assuming that $\Delta_{ij} = \hbar |\Delta \Omega_i - \Delta \Omega_j| \gg J_{ij}$ is satisfied, then the $\hat{\mathcal{H}}_{\text{mix}}^{XY}$ term in Eq. (1) turns non-secular and a free evolution is in consequence achieved: spins evolve in isolation from one another. Conversely, to optimize a transfer of polarization between sites, the longitudinal interaction needs to be erased –for example by using radiofrequency (rf)-based methods that refocus the shifts of all spins [14]. The system will then evolve with a nearly pure mixing Hamiltonian $\hat{\mathcal{H}}_{\text{mix}}$; as this

Hamiltonian connects all possible spin pairs, an initial local excitation will spread over the full spin network. To avoid this and confine the spin network topology to a selected, optimized spin transfer pathway, one needs to effectively disconnect spins that do not belong to this sub-network. We achieve this by exploiting the chemical shift differences among the sites involved; specifically, by implementing a sequence whereby the \hat{H}_{mix} evolution is stroboscopically interrupted with free evolution periods driven by \hat{H}_Z (Fig. 1a). If periods of coupled and free evolutions are alternated n -times, and the free evolution time, τ_{free} , is adjusted to a common multiple of the inverses of the chemical shift differences Δ_{ij} between the spins of the pathway (i.e. $\tau_{\text{free}} = 2\pi n_{ij}\hbar/|\Delta_{ij}|$, where n_{ij} is a positive integer), only the i and j spins in the pathway experience a coherent \hat{H}_{mix} -driven buildup. And only between these spins the PST proceeds coherently. By contrast all other pathways are dephased by the free evolution, leading to their effective decoupling. This

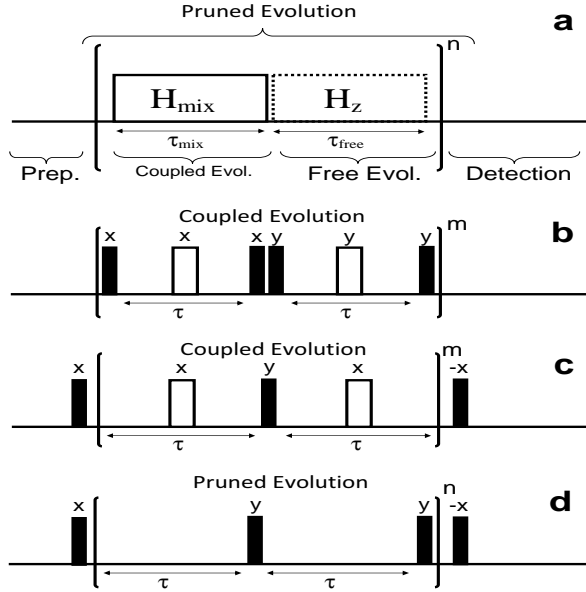


Figure 1: Quantum evolution schemes for achieving perfect state transfers (PSTs) in homonuclear NMR systems. (a) Sequence delivering PST when $\hat{H}_{\text{mix}} = \hat{H}_{\text{mix}}^{XY}$ and a suitable number n of repetitions is used. (b, c) NMR mixing sequences to generate an effective XY Hamiltonian in liquid state systems, starting from a spin-spin Ising-type interaction [9]. m is the number of loops defining the resulting $\hat{H}_{\text{mix}}^{XY}$ Hamiltonian. (d) Alternative sequence incorporating quantum evolutions under the combined effects of \hat{H}_{mix} and \hat{H}_Z Hamiltonians, capable of generating a PST between specific homonuclear offsets based on an Ising spin-spin interaction. Solid lines represent $\pi/2$ pulses; hollow boxes are π pulses.

decoupling turns more effective by reducing the \hat{H}_{mix} evolution time τ_{mix} because it increases the detuning between the selected spins and the remaining ones as

can be observed by the zero-order average Hamiltonian $(\tau_{\text{free}}\hat{H}_Z^{\neq i \neq j} + \tau_{\text{mix}}\hat{H}_{\text{mix}}) / (\tau_{\text{free}} + \tau_{\text{mix}})$, where $\hat{H}_Z^{\neq i \neq j}$ is a Zeeman Hamiltonian for the remaining spins. Moreover, by judiciously turning on-and-off transfers within any two/three qubits, one can control by PSTs between arbitrarily chosen pairs of spins even throughout complex spin network topologies. From a quantum-mechanical standpoint this can be interpreted as a successive establishment of decoherence-free subspaces, where the only allowed dynamics occurs within a confined region of the spins' Hilbert space [15]. Indeed the repetitive interruption of \hat{H}_{mix} with the strong \hat{H}_Z interactions can be shown equivalent to a stroboscopic measurement of local variables [16]. This results in a dynamical Quantum Zeno Effect [17] that freezes certain portions of the internal quantum dynamics, and delivers a nearly ideal PSTs. This is by contrast to standard PST implementations, that rely on concatenated SWAP gates (like those afforded by selective pulses) to achieve similar goals –but via more demanding, local manipulations [8].

In liquid-state homonuclear systems at high fields, $|\Delta_{ij}| \gg J_{ij}$, and the intrinsic $\hat{H}_{\text{mix}}^{XY}$ terms will be truncated. Although not naturally available, such flip-flop couplings can be reintroduced in an average way, by toggling the usual high-field Ising J -interaction, $\hat{H}_{\text{mix}}^{ZZ} = \sum_{i \neq j} J_{ij} \hat{I}_i^z \hat{I}_j^z$, into an effective XY Hamiltonian. Rotating the $\{I_\alpha\}_{\alpha=x,y,z}$ states at a high rate with respect to the relevant interactions as schematized in Fig. 1b, transforms the averaged Ising Hamiltonian, into an effective $\hat{H}_{\text{mix}}^{XY}$ [9]. Fig. 1c shows an alternative sequence, capable of achieving the same Hamiltonian but in an experimentally more robust manner. This latter scheme still requires appending a free evolution period τ_{free} , tuned to the inverse shift difference Δ_{ij} between the pair of sites among which one intends the PST. Instead of inserting these delays explicitly, we modified the sequence in Fig. 1c to impose an offset dependence, which truncates all J_{ij} effects except for those spin-pairs for which the τ^{-1} inverse interval is a common multiple of the chemical shift differences $\Delta_{ij} = \hbar(\Delta\Omega_i - \Delta\Omega_j)$. This alternative (Fig. 1d), which was experimentally the most robust variant assayed, effectively connects coupled spins in a pathway if they fulfill $\tau = 2\pi n_{ij}\hbar/|\Delta_{ij}|$, while dephasing the transfer between all other pairs of spins. Assuming that $|\Delta_{ij}| \gg J_{ij}$, only the targeted spin pairs undergo an effective PST.

Numerical simulations.– The concepts just mentioned were numerically tested to explore, their usefulness for performing PSTs within an ideal spin network. Specifically, we sought to inquire into the efficiency of the truncated XY mixing Hamiltonian to support long-range transfers between non-neighboring spins; both directly, as well as through numerous pair-wise stop-overs involving intermediate spins. For concreteness, we focused on the six-spin system of the L-leucine's ^{13}C backbone; whose chemical

shifts $\Delta\nu_i = \Delta\Omega_i/2\pi$ and J -couplings, obtained experimentally by NMR, are listed in Fig. 2. Numerical simulations of sequence 1a with $\hat{H}_{\text{mix}} = \hat{H}_{\text{mix}}^{XY}$, $\hat{H}_{\text{free}} = \hat{H}_Z$ are shown in Figs. 2a-d. These plots describe the fidelity of PSTs solely as a function of the targeted qubits' $|\uparrow\rangle_z$ -probability. Such description is made possible thanks to the fact that the total $\sum_i \hat{I}_i^z$ angular momentum is a constant of motion: The transfer of a qubit state on i throughout a network can thus be gauged if, given an initial state where $|i\rangle = |\uparrow\rangle_z$ and all remaining spins are $|\downarrow\rangle_z$, the latter's evolution in time is followed [4]. The top and bottom panels of Fig. 2 focus on such description assuming two different PST targets, whereas its left/right-hand sides compare the differences between selectively-transferred and normal $\hat{H}_{\text{mix}}^{XY}$ pathways. Figs. 2a-b illustrate the behavior of the spin up probabilities that starting in site C_α , undergoes a fully spin-spin coupled or a PST-selective XY evolution between the sites C_α and C_β . The excellent selectivity of the latter choice is evidenced by the long-term, coherent nature of the oscillations. Fig. 2c illustrates a different aspect of the PST, whereby the initial excitation is localized at the CO carbonyl site and, by successively selecting a train of suitable conditions $\tau_{\text{free}} = 2\pi\hbar/\Delta_{ij}$, this is subsequently passed through all the sites in the main molecular chain until reaching the end C_{δ_1} site. In other words, by selecting $\tau_{\text{free}} = 2\pi\hbar/\Delta_{\text{CO},\alpha}$ one can do a PST to the C_α site; once this state transfer is maximized one can then set $\tau_{\text{free}} = 2\pi\hbar/\Delta_{\alpha,\beta}$ and transfer it to site C_β , and onwards with successive steps until the initial state has been transferred to the δ_1 site. Although relatively time consuming, this step-by-step transfer is realized with high efficiency and without accessing δ_2 , owing to the method's high selectivity. This is in stark contrast with the very complex behavior observed when allowing the spin system to evolve under a pure $\hat{H}_{\text{mix}}^{XY}$ evolution (Fig. 2d). Similar curves are obtained when the initial excitation is on the other spins. PST between arbitrary sites in a branched network is thus achieved, without having to address the individual qubits selectively.

Experiments.— The new PST approach and its associated features were tested using liquid state ^{13}C NMR as a sort of “quantum simulator”. These experiments were carried out at 298 K and 11.7 T, using $\text{U-}^{15}\text{N}$, ^{13}C -Leu-FMOC dissolved in CDCl_3 as test case. The measured chemical shifts (in kHz referenced to $\delta_{\text{TMS}} = 0$), the J -couplings, as well as the spin-coupling topology, were summarized in Fig. 2. Figure 3 schematizes the actual pulse sequence assayed on this test system, together with comparisons between polarization evolutions observed for different initial conditions and different pathways as building blocks for piecewise transfers; also shown are calculations of the expected behavior. To better gauge this comparison we prepared an initial, local excitation, applying a selective $\pi/2$ pulse on the source site, which turned the initial magnetization of the selected spin to a perpendicular axis of the static magnetic

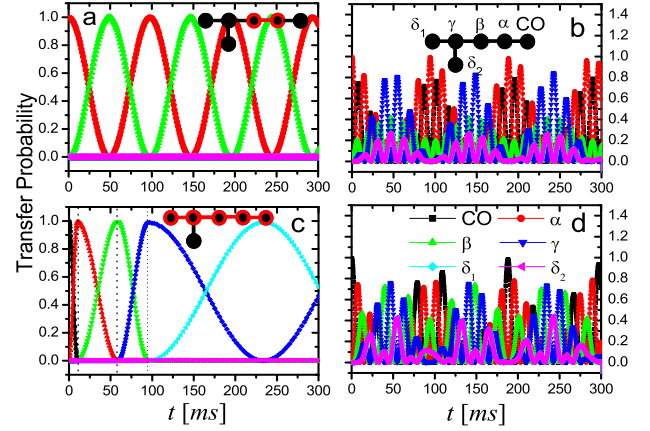


Figure 2: (color online) Numerical simulations for perfect state transfers throughout different sites of the ^{13}C L-leucine molecule backbone. \hat{H}_{mix} was assumed a perfect $\hat{H}_{\text{mix}}^{XY}$, and $\hat{H}_{\text{free}} = \hat{H}_Z$ was selected with $\tau_{\text{mix}} = 0.3 \text{ ms} \ll 2\pi\hbar/J$. (a) PST between the spin sites α and β by selecting $\tau_{\text{free}} = 2\pi\hbar/\Delta_{\alpha\beta}$. (b) Counterpart evolution starting also from site α , but acted upon by a pure $\hat{H}_{\text{mix}}^{XY}$ evolution. (c) Step-wise PST starting from an initial excitation on the CO spin and concluding in the δ_1 spin. $\tau_{\text{free}} = 2\pi\hbar/\Delta_{ij}$ was chosen to effectively reduce the system to a series of two-spin transfers, proceeding throughout the backbone. (d) Counterpoint evolution expected for all spins in the system starting from an initial CO site excitation, but proceeding under the action of an unfiltered $\hat{H}_{\text{mix}} = \hat{H}_{\text{mix}}^{XY}$ coupled evolution. Bottom: Scheme of the spin network and their parameters obtained from NMR experiments.

field. Then, a non-selective $\pi/2$ pulse restores back to the z axis the source spin, while all the other spin magnetizations turn transverse to the static field. These magnetizations were then promptly dephased by applying a field gradient pulse. This source of polarization, which is in a single site, is then rotated to the $-y$ axis by a non-selective pulse, and followed by a mixing sequence akin to that in Fig. 1d. The transferred polarizations were observed at times $t = 2n\tau$. The rf carrier frequency was set on-resonance with C_β ; all polarizations thus appeared evolving in a rotating frame that precessed with frequency $\Delta\Omega_\beta$. While these examples illustrate the good PST performance for longitudinal polarizations transfers which are the equivalent of an excitation transfer probabilities, a complete performance test within NMR ensemble quantum computation would require the incorporation of pseudo-pure states into this kinds of manipulations [18].

The main effects of the selective PST are observed very well—even if some undesired residual magnetization from non-source spins survived the initial purging process, and despite the limited performance that our non-selective pulses could achieve given the maximal 19 kHz radiofrequency fields achievable in our system. In Fig. 3a τ was

set as $0.71 \text{ ms} \simeq 2\pi\hbar/|\Delta_{\alpha\beta}|$ producing a polarization transfer between sites C_α and C_β , while effectively decoupling the remaining ^{13}C - ^{13}C interactions. Figs. 3 b-c show additional examples of pairwise PSTs. Values of $\tau = 3.88 \text{ ms} = 8 \times 2\pi\hbar/|\Delta_{\beta\gamma}| \simeq 2\pi\hbar/|\Delta_{\gamma,\delta_2}|$ favored the selective transfer from site C_β to carbon C_γ and on to site C_{δ_2} (Fig. 3b); choosing δ_1 instead of δ_2 , $\tau = 4.81 \text{ ms}$, optimized a similar transfer but for the $C_\beta \rightarrow C_{\delta_1}$ case (Fig. 3c). Though the chosen times τ were not perfectly commensurate with their ideal values, the functionality of the method is evident. And the overall agreement with numerical simulations that consider the entire sequence (lines in Fig. 3) is excellent.

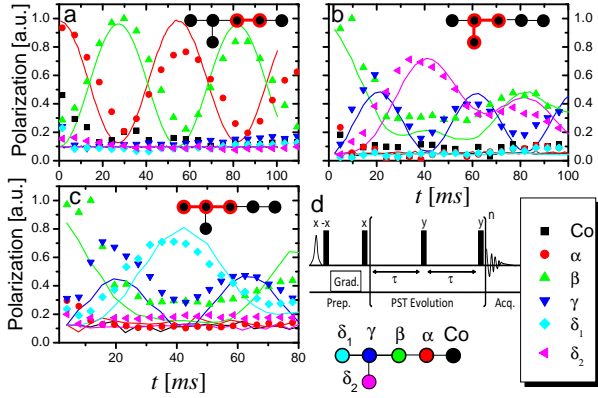


Figure 3: (color online) NMR experiments (points) and numerical expectations (lines) for selective state transfers implemented for different situations by using the NMR pulse sequence illustrated in the lower right corner –derived in turn from Fig. 1d. (a) An initial excitation on α is transferred to the β spin. (b) An initial C_β excitation is optimally transferred to δ_2 via the $\beta - \gamma - \delta_2$ pathway. (c) An initial C_β excitation is selectively transferred to δ_1 via the $\beta - \gamma - \delta_1$ pathway.

Conclusions.— A method for achieving a directional, perfect state transfer within a branched spin network without individual manipulation of the spins, has been proposed and demonstrated. The method requires knowledge of system parameters such as the chemical shifts, but does not need selective qubit manipulations. As a result the method is general and independent of the system size in contrast to methods based on selective manipulations where the number of individual manipulations grows roughly exponentially with the system size [8]. Selectively information transfers among proximal or distal qubits regardless of the spin network topology was then demonstrated, by engineering a Hamiltonian that exploits the two non-commuting contributions to the system’s evolution: one involving a pure XY interaction, and the other a pure Zeeman evolution. Alternatives for generating such selective XY interactions by means of manipulating Ising couplings, were also shown, acting by establishing decoherence-free subspaces where complete PSTs

between the targeted spins can occur, while effectively “pruning” away those qubits where no excitation transfer is required. While the experimental performance of the approach was illustrated with PSTs of longitudinal polarizations, the method can, in general, provide a selective, specific transfer pathway in a system of many interacting spins for arbitrary initial states for the source spin. Moreover, by dividing a complex spin network into smaller sub-ensembles, this approach provides an excellent starting point for performing other large quantum systems using solely global manipulations that exploit the time-domain quantum interferences. Some of these will be discussed in further detail in upcoming studies.

This work was made possible by a Fundación Antorchas – Weizmann Institute Cooperation (grant #2530), by CONICET, by a Helen and Kimmel Award for Innovative Investigations, as well as by the generosity of the Perlman Family Foundation. GAA and EPD thank the Alexander von Humboldt Foundation for Research Scientist Fellowships.

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